

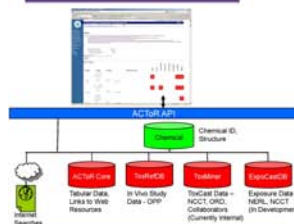


EPA NCCT Databases and Knowledgebases: ACToR, DSSTox, ToxRefDB, ToxMiner, ExpoCastDB, and VT-KB

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ACToR Aggregated Computational Toxicology Resource



- Compile all publicly available information on environmental chemicals
 - One-stop shop
 - Make previously hard-to-access data transparent (e.g. from OPP)
- Make data available for downloading, data mining
 - Available through data.gov
 - Entire DB can be downloaded and installed locally
- Make it easy to see data gaps
 - Provides resource for EPA testing programs
- Make it widely used
 - over 2000 regular users

<http://actor.epa.gov>

DSSTox Distributed Structure-Searchable Toxicity Database Network



- Public resource for high quality chemical structures and chemical annotation in association with toxicity data
- Publishes summarized activity representations for structure-activity modeling
- Structure-browser for structure analog searching across resources
- Promoting chemical information reporting standards in toxicology
- Providing chemical information management & cheminformatics foundation for ToxCast and Tox21 projects

<http://www.epa.gov/ncct/dsstox>

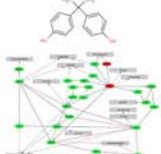
ToxRefDB Toxicity Reference Database



- Extracted from OPP internal DB
- Relational phenotypic/toxicity database
- Provides in vivo anchor for ToxCast predictions
- Three study types
 - Chronic/Cancer rat and mouse (Martin, et al. EHP 2008)
 - Rat multigenerational Reproduction (Martin, et al. submitted)
 - Rat & Rabbit developmental (Knudsen, et al. internal review)
- Two types of synthesis
 - Supervised (common individual phenotypes)
 - Unsupervised (machine based clustering of phenotype patterns)

<http://actor.epa.gov/toxrefdb>

ToxMiner ToxCast Database



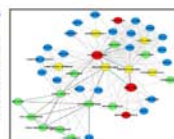
- All ToxCast Data
- Links
 - Chemicals
 - Assays
 - Genes
 - Pathways
 - Endpoints
- Allows data analyses
 - Statistical associations
 - Biologically drive data mining

ExpoCastDB EPA Exposure Database



- Consolidate and link human exposure and exposure factor data for chemical prioritization and toxicity testing
 - Disseminate measurements from human exposure studies
 - Facilitate linkages with toxicity data and product usage data
 - Facilitate application of informatics tools for large-scale, multidimensional data analysis
- Define exposure domain with formal representation of key concepts and relationships
- Provide basic user functions
 - Visualization (e.g., scatterplots, probability plots, goodness-of-fit)
 - Estimate distributional parameters
 - Download customized datasets

VT-KB Virtual Tissues Knowledgebase



1. VT Knowledgebase (VT-KB) support the development of in silico models to predict multicellular behaviors of specific biological systems including developing embryo (v-Embryo™) and chronic liver injury (v-Liver™).
2. Extract and organize relevant facts from the scientific literature and other sources of information
3. Provide interactive graphical tools to analyze/curate the literature and navigate the VT-KB: c-Mantic (standalone) and ToxPlover (web based)

<http://www.epa.gov/ncct/v-Embryo>
http://www.epa.gov/ncct/Virtual_Liver

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